Analysis output: all-atom contacts and geometry for pembrolizumab_abb2_1FH.pdb

Duke Biochemistry
Duke University School of Medicine

Summary statistics

All-Atom Contacts	Clashscore, all atoms:	0.57		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	6	3.08%	Goal: <0.3%
	Favored rotamers	181	92.82%	Goal: >98%
	Ramachandran outliers	1	0.44%	Goal: <0.05%
	Ramachandran favored	221	97.36%	Goal: >98%
	Rama distribution Z-score	-1.59 ± 0.53		Goal: abs(Z score) < 2
	MolProbity score^	1.19		99th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 1840	0.00%	Goal: 0%
	Bad angles:	9 / 2497	0.36%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 10	20.00%	Expected: ≤1 per chain, or ≤5%
Low-resolution Criteria	CaBLAM outliers	3	1.3%	Goal: <1.0%
	CA Geometry outliers	0	0.00%	Goal: <0.5%
Additional validations	Chiral volume outliers	0/269		
	Waters with clashes	0/0	0.00%	See UnDowser table for details

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

Key to table colors and cutoffs here:

Multi-criterion visualizations

View in KiNG | View in NGL | Download (961 Kb)

View (279 Kb)

View (2.8 Kb)

Single-criterion visualizations

- **Clash list** (256 bytes): View
- **Ramachandran plot kinemage** (419 Kb): View in KiNG | View in NGL | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Ramachandran distribution Z-score analysis** (12 Kb): View
- **Chiral volume report** (788 bytes): View
- **Cβ deviation scatter plot** (18 Kb): View in KiNG | View in NGL | Download

Continue >